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An Integrated Methodology for Design of Tailor-Made Blended Products: Biofuels and Bio-Based Lubricants

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323 (Convention Center)

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The demand for bio-based products has been growing in recent years due to increasing concerns about the environment, resource depletion, and/or sustainability. Bio-based products can be designed by blending of conventional materials (e.g. fossil fuels) with other chemicals produced from renewable resources, such as biomass, reducing thereby the fossil fuel consumption and amount of pollutants released into the environment, and increasing the product safety. A tailor-made bio-based blended product is a mixture of several chemicals and designed to match specific product attributes. The most challenging task and critical step in tailor-made bio-product design is to identify and select the appropriate chemicals to be used as building blocks for the blend. At the initial stage, searching for the blend chemicals (additives) is uncertain and involves a very large search space. Therefore, it is important to have a method to systematically and efficiently reduce the search space within which the solution to the blending problem may be found. Once the candidate chemicals have been identified, their optimal compositions in the blend are determined, while still matching the target properties.

In this study, an integrated methodology for design of tailor-made bio-based blended products is presented. The methodology is able to find the composition of optimal blended bio-based products, and consists of two stages; The first stage is product design, where a computer-aided methodology is implemented to identify and evaluate the most promising blend candidates. Then, in the second stage, the blend attributes are validated experimentally or with rigorous simulation models. The first stage consists of four tasks. The first task is to define the design problem, where the product needs are identified, translated into target properties and given target values. In the second task, the required target property models are retrieved from a property model library developed specifically for bio-based blended products. The property model library stores the pure and mixture property models with their parameters. Also, a chemical database, which is one of the important tools in this integrated methodology, has been developed. This database stores the pure compounds which originate from renewable and non-renewable sources with their properties that may be used as building blocks in the blend design. In the third task, the blend problem is solved using a blend design algorithm to find the blends that best match the design targets. In this way, the amount of bio-based chemicals in the blend can be controlled and adjusted. This algorithm employs a decomposition based solution strategy to screen for the feasible blend candidates, thus reducing the search space in a systematic way. The result is a set of blends that match the desired targets, the compositions, values of the target properties and information about their miscibility. Finally, the mixture target property values are verified by rigorous models for the properties and mixtures that require it. Here, collection of data in the database helps in verifying the predicted blend properties.

The application of this systematic methodology is highlighted through case studies related to the design of sustainable and better performing blended gasoline and lubricants with bio-based chemicals. The objective of the case studies is to identify suitable bio-based chemicals as well as the blended products where they can be used.

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